International Tables For Crystallography Volume B Reciprocal Space

International Tables for Crystallography are no longer available for purchase from Springer. For further information please contact Wiley Inc. (follow the link on the right hand side of this page). This brief teaching edition is a condensed, inexpensive version of Volume A of International Tables for Crystallography. It consists of: complete descriptions of the 17 plane groups, useful for the teaching of symmetry 24 selected space-group examples, of varying complexity and distributed over all seven crystal systems those basic text sections of Volume A that are necessary for the understanding and handling of space groups (Parts 1, 2, 3 and 5). The purpose of the teaching edition is threefold: It should provide a handy (and inexpensive) tool for researchers and students wishing to familiarize themselves with the use of the space-group tables in Volume A. It is designed for use in classroom teaching, and with this aim in mind the price has been kept as low as possible. In order to achieve this, the material has been reprinted from Volume A without any changes, except for pagination. It may serve as a laboratory handbook because the 24 examples include most of the frequently occurring space groups, for both organic and inorganic crystals. The fifth edition of the brief teaching edition has been reviewed by M. Warren [Mineral. Mag. (2003). 67, 826-827].

Until the 1970s all materials studied consisted of periodic arrays of unit cells, or were amorphous. A new class of solid state matter called aperiodic crystals has since been uncovered. It is a long range ordered structure, but without lattice periodicity. It is found in a wide range of materials: organic and anorganic compounds, minerals (including a substantial portion of the earths crust), and metallic alloys, under various pressures and temperatures. Because of the lack of periodicity, the usual techniques for the study of structure and physical properties no longer work, and new techniques have to be developed. This book deals with the characterisation of the structure, the structure determination and the study of the physical properties, especially dynamical and electronic properties of aperiodic crystals. The treatment is based on a description in a space with more dimensions than three, the so-called superspace. This allows us to generalise the standard crystallography and to look differently at the dynamics. The three main classes of aperiodic crystals, modulated phases, incommensurate composites and quasicrystals are treated from a unified point of view, which stresses similarities of the various systems. The book assumes as a prerequisite a knowledge of the fundamental techniques of crystallography and the theory of condensed matter, and covers the literature at the forefront of the field. Since the first edition of this book in 2007, the field of aperiodic crystals has developed considerably, with the discovery of new materials and new structures. Progress has been made in structure determination, in the interpretation and understanding of the structural characteristics and in the calculation of electrons and phonons. This new edition reflects these new developments, and it includes discussions of natural quasicrystals, incommensurate magnetic and multiferroic structures, photonic and mesoscopic quasicrystals. The second edition also includes a number of new exercises that give the reader an opportunityt to check their understanding of the material.

The International Tables for Crystallography are jointly published with the International Union of Crystallography. Each print

volume can be purchased individually. In addition the complete set of Vol A-G is available both in print and online (see right hand column). International Tables for Crystallography, Volume E, Subperiodic groups covers the seven frieze groups, the 75 rod groups and the 80 layer groups. The information tabulated for these groups is identical in format and content as that given for the 230 space groups in Volume A. In addition, scanning tables are given for each of the 230 space groups. These scanning tables give the largest subgroup of the space group that leaves the given plane invariant. The use of the scanning tables is shown in determining the symmetry of domain walls. Volume E has been reviewed by R. Gould (Crystallography News, No. 85, June 2003, p. 13). International Tables for personal use can be purchased at a discount. Contact Customer Service for further information and to place an order.

Offers a rigorous treatment of the theory of crystallography and detailed descriptions of experimental applications in a wide range of sciences, including computational aspects, protein crystallography and crystal physics.

International Tables for Crystallography are no longer available for purchase from Springer. For further information please contact Wiley Inc. Since the mid-thirties the successive editions of the International Tables for Crystallography, with slight variations in name, have been the indispensable companions of all crystallographers and most other scientists concerned with the structure of materials: biochemists, chemists, metallurgists, mineralogists and physicists. The present Volume C is the third in the series that constitutes the current editions, and replaces Volumes II, III and IV of the previous edition. The main contents are crystal geometry, diffraction geometry, preparation of specimens, production and properties of radations, determination of lattice parameters, measurement and interpretation of diffracted intensities, refinement of structural parameters, basic structural features, and precautions against radiation injury. Volume C thus supplements Volume A (Space-Group Symmetry) and Volume B (Reciprocal Space).

This sixth edition of what was previously known as the Brief Teaching Edition of Volume A provides an introduction to the basic crystallographic data for space groups found in Volume A, for symmetry relations between space groups in Volume A1 and for subperiodic groups in Volume E of International Tables for Crystallography, to magnetic space groups and to the symmetry database that forms part of International Tables Online at https://it.iucr.org. It is designed for graduate students and young researchers who are new to the field of crystallographic symmetry, and includes many illustrative examples to help readers to understand and use these different kinds of information. Selected tables of symmetry data from the full volumes in the series are also included, making this a handy aid for classroom teaching. References are also provided to further specialized sources for those who need to go deeper into the subject and to textbooks for those who need more background information.

The atomic arrangements in condensed matter play an ever increasing role in many areas of science and technology - Materials Science and Engineering, Chemistry, Physics, Geology, Biology and Electrical, Civil, Mechanidtl and Chemical Engineering. Exciting discoveries in these fields in this century often stemmed from studies of these arrangements using diffraction: the structure and functions of DNA and other biological molecules, the configuration of polymer chains, the crystalline nature of metals and their imperfections, semiconductors and

insulators, and -the links between their structures, their defects and material properties, and the interaction between materials and the environment. The broad, interdisciplinary character of diffraction studies makes them particularly exciting. With new tools such as the high-resolution electron microscope, new detectors, new techniques (such as EXAFS and glancing angle diffraction) and the new sources, the horizons of this field greatly expanded in the 1950's and 60's. Pulsed neutron sources and high intensity storage rings that came on the scene in the late 70's have opened up possibilities for new study to such vast horizons that it is hard to sit here writing this - there's so much to be done! Within the walls bounding each field of science or engineering, diffraction and structure is only one specialty. It is too easy for this topic to be developed in such a narrow way that sight is lost of the basic principles and broad possibilities.

International Tables for Crystallography is the definitive resource and reference work for crystallography and structural science. Each of the eight volumes in the series contains articles and tables of data relevant to crystallographic research and to applications of crystallographic methods in all sciences concerned with the structure and properties of materials. Emphasis is given to symmetry, diffraction methods and techniques of crystal-structure determination, and the physical and chemical properties of crystals. The data are accompanied by discussions of theory, practical explanations and examples, all of which are useful for teaching. International Tables for Crystallography comprises more than 6,000 pages including nearly 2,000 pages of symmetry tables which are vital for the analysis of crystal structures: Volume A: Space-group symmetry, 5e Volume A1: Symmetry relations between space groups, 2e Volume B: Reciprocal space, 3e Volume C: Mathematical, physical and chemical tables, 3e Volume D: Physical properties of crystals Volume E: Subperiodic groups, 2e Volume F: Crystallography of biological macromolecules, 2e Volume G: Definition and exchange of crystallographic data This edition includes a new edition of Volume F, making International Tables the most up-to-date, dynamic, and comprehensive reference work available to crystallographers, and to all those who use crystallography across a wide range of fields.

International Tables for Crystallography: Space-group symmetryInternational Tables for Crystallography, Volume BReciprocal SpaceSpringer Science & Business Media

International Tables for Crystallography are no longer available for purchase from Springer. For further information please contact Wiley Inc. (follow the link on the right hand side of this page). The purpose of Volume C is to provide the mathematical, physical and chemical information needed for experimental studies in structural crystallography. The volume covers all aspects of experimental techniques, using all three principal radiation types, from the selection and mounting of crystals and production of radiation, through data collection and analysis, to interpretation of results. As such, it is an essential source of information for all workers using crystallographic techniques in physics, chemistry, metallurgy, earth sciences and molecular biology.

International Tables for Crystallography is the definitive resource and reference work for crystallography and structural science. Volume A of the series, Space-group symmetry, contains diagrams and tables of data for the 17 plane groups, the 230 space groups and the 32 crystallographic point groups.This new edition is edited by M. I. Aroyo and has been extensively updated and revised. Part 1 of the volume provides an introduction to space-group symmetry. It includes chapters on groups, crystallographic and space-group symmetry, descriptions of space groups, coordinate-system transformations and methods of space-group determination. The final chapter provides a useful introduction to topics treated in more depth in Volumes A1 and E of the series. The chapters in this part have been written with teaching in mind, and will prove invaluable for undergraduates or graduates wishing to learn about symmetry in crystallography, while providing a clear introduction to the topic for researchers from other disciplines. Part 2 of the volume presents the diagrams and tables of plane- and space-

group data. The layout of the tables of data, the symbols used in the diagrams and the classification of the space groups are explained in a useful guide. Together these form an essential resource not only for professional crystallographers, but also for chemists, physicists, mineralogists, biologists and material scientists who employ crystallographic methods and who are concerned with the structure and the properties of crystalline materials. Part 3 treats more advanced topics on space-group symmetry, and covers crystal lattices, point groups and crystal classes, space-group symbols and their use, lattice complexes, normalizers of space groups, and magnetic subperiodic groups and magnetic space groups. There are eight new chapters in this 6th edition of Volume A, and five chapters have been revised. The layout of the space-group tables has been simplified as the sub- and supergroup data are now available in Volume A1, and there are new general-position diagrams for the cubic space groups. Additional diagrams showing tilted, perspective views of some of the more complex cubic space groups are also provided.

International Tables for Crystallography Volume G, Definition and exchange of crystallographic data, describes the standard data exchange and archival file format (the Crystallographic Information File, or CIF) used throughout crystallography. It provides in-depth information vital for small-molecule, inorganic and macromolecular crystallographers, mineralogists, chemists, materials scientists, solid-state physicists and others who wish to record or use the results of a single-crystal or powder diffraction experiment. The volume also provides the detailed data ontology necessary for programmers and database managers to design interoperable computer applications. The accompanying CD-ROM contains the CIF dictionaries in machine-readable form and a collection of libraries and utility programs. This volume is an essential guide and reference for programmers of crystallographic software, data managers handling crystal-structure information and practising crystallographers who need to use CIF.

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The general purpose of Volume B of the International Tables for Crystallography is to present the user/reader with competent and useful accounts of the numerous aspects of reciprocal space in crystallographic research. After an introductory chapter, Part 1 presents the reader with an account of structure factor formalisms, an extensive treatment of the theory, algorithms and crystallographic applications of Fourier methods and a treatment of symmetry in reciprocal space. In Part 2 of the volume these general accounts are followed by detailed expositions of crystallographic statistics, direct methods, Patterson techniques, isomorphous replacement and anomalous scattering, and treatments of the role of electron microscopy and diffraction in crystal structure determination. Part 3 deals with applications of reciprocal space to molecular geometry and `best' plane calculations; it contains a treatment of the principles of molecular graphics and modelling and their applications, and concludes with the presentation of a convergence-acceleration method, of importance in the computation of approximate crystal potentials. The fourth Part contains treatments of various diffuse scattering phenomena arising from crystal dynamics, disorder and low dimensionality (liquid crystals), and an exposition of the underlying theories and/or experimental evidence. The volume concludes with an introductory treatment of the theory of interaction of radiation with matter, the so-called dynamical theory. Insofar as it was possible, effects due to all three major diffraction techniques (X-rays, neutrons and electrons) are considered. The volume is a vital addition to the library of scientists engaged in crystal structure determination, crystallographic computing, crystal physics and other fields of crystallogaphic research. Graduate students specializing in crystallography will find much material suitable for self study and a rich source of references to the relevant literature.

This comprehensively revised – essentially rewritten – new edition of the 1990 edition (described as "extremely useful" by MATHEMATICAL

REVIEWS and as "understandable and comprehensive" by Scitech) guides readers through the dense array of mathematical information in the International Tables Volume A. Thus, most scientists seeking to understand a crystal structure publication can do this from this book without necessarily having to consult the International Tables themselves. This remains the only book aimed at non-crystallographers devoted to teaching them about crystallographic space groups. Reflecting the bewildering array of recent changes to the International Tables, this new edition brings the standard of science well up-to-date, reorganizes the logical order of chapters, improves diagrams and presents clearer explanations to aid understanding Clarifies, condenses and simplifies the meaning of the deeply written, complete Tables of Crystallography into manageable chunks Provides a detailed, multi-factor, interdisciplinary explanation of how to use the International Tables for a number of possible, hitherto unexplored uses Presents essential knowledge to those needing the necessary but missing pedagogical support and detailed advice – useful for instance in symmetry of domain walls in solids

This book invites you on a systematic tour through the fascinating world of crystals and their symmetries. The reader will gain an understanding of the symmetry of external crystal forms (morphology) and become acquainted with all the symmetry elements needed to classify and describe crystal structures. The book explains the context in a very vivid, non-mathematical way and captivates with clear, high-quality illustrations. Online materials accompany the book; including 3D models the reader can explore on screen to aid in the spatial understanding of the structure of crystals. After reading the book, you will not only know what a space group is and how to read the International Tables for Crystallography, but will also be able to interpret crystallographic specifications in specialist publications. If questions remain, you also have the opportunity to ask the author on the book's website.

International Tables for Crystallography is the definitive resource and reference work for crystallography and structural science. Each of the eight volumes in the series contains articles and tables of data relevant to crystallographic research and to applications of crystallographic methods in all sciences concerned with the structure and properties of materials. Emphasis is given to symmetry, diffraction methods and techniques of crystal-structure determination, and the physical and chemical properties of crystals. The data are accompanied by discussions of theory, practical explanations and examples, all of which are useful for teaching. International Tables for Crystallography provides access to the content of the full set (6000 pages) of all the Volumes A to G including A1 in pdf format and also provides access to the International Tables Online site hosted by the International Union of Crystallography. The International Tables Online site contains the full text of the series as both pdf and richly interlinked html, along with many innovative features and additional resources. The advanced search facility enables sophisticated searches to be performed across all the volumes, across selected volumes and across International Tables Online and Crystallography Journals Online. The International Tables for Crystallography includes nearly 2,000 pages of symmetry tables which are vital for the analysis of crystal structures, and which feature extensive linking between sub- and supergroups. The contents can be browsed by volume, across the 8 volumes below: Volume A: Space-group symmetry, 5e Volume A1: Symmetry relations between space groups Volume B: Reciprocal space, 3e Volume C: Mathematical, physical and chemical tables, 3e Volume D: Physical properties of crystals Volume E: Subperiodic groups Volume F: Crystallography of biological macromolecules Volume G: Definition and exchange of crystallographic data Within each volume, users can navigate to view a full chapter, a section or sub-section, or a single figure or table. Cross-references are included between chapters of related interest. With new editions of volumes E and A1 to be added in 2010, and further new editions to be added in subsequent years, the International Tables Online truly represents the most up-to-date, dynamic, and comprehensive reference work available to crystallographers, and to all those who use crystallography across a wide range of fields.

International Tables for Crystallography are no longer available for purchase from Springer. For further information please contact Wiley Inc. The purpose of Volume C is to provide the mathematical, physical, and chemical information needed for experimental studies in structural crystallography. This new edition features two completely new chapters, on reflectometry and neutron topography. More than half of the text has been revised and updated, and there are extensive updates and corrections to tabular material. Volume C covers all aspects of experimental techniques, using all three principal radiation types, from the selection and mounting of crystals and production of radiation through data collection and analysis to interpretation of results. Audience: The volume is an essential source of information for all workers using crystallographic techniques in physics, chemistry, metallurgy, earth sciences, and molecular biology.

International Tables for Crystallography is the definitive resource and reference work for crystallography and structural science. Each of the eight volumes in the series contains articles and tables of data relevant to crystallographic research and to applications of crystallographic methods in all sciences concerned with the structure and properties of materials. Emphasis is given to symmetry, diffraction methods and techniques of crystal-structure determination, and the physical and chemical properties of crystals. The data are accompanied by discussions of theory, practical explanations and examples, all of which are useful for teaching. International Tables for Crystallography comprises 6,000 pages including nearly 2,000 pages of symmetry tables which are vital for the analysis of crystal structures: Volume A: Space-group symmetry, 5e Volume A1: Symmetry relations between space groups, 2e Volume B: Reciprocal space, 3e Volume C: Mathematical, physical and chemical tables, 3e Volume D: Physical properties of crystals Volume E: Subperiodic groups, 2e Volume F: Crystallography of biological macromolecules Volume G: Definition and exchange of crystallographic data This edition includes new editions of Volumes A1 and E, making International Tables the most up-to-date, dynamic, and comprehensive reference work available to crystallographers, and to all those who use crystallography across a wide range of fields.

This textbook is a complete and clear introduction to the field of crystallography. It includes an extensive discussion on the 14 Bravais lattices and their reciprocals, the basic concepts of point- and space-group symmetry, the crystal structure of elements and binary compounds, and much more. The purpose of this textbook is to illustrate rather than describe "using many words" the structure of materials. Even readers who are completely unfamiliar with the topic, but still interested in learning how the atoms are arranged in crystal structures, will find this book immensely useful. Each chapter is accompanied by exercises designed to encourage students to explore the different crystal structures they are learning about. The solutions to the exercises are also provided at the end of the book.

The precise knowledge of the structure of biological macromolecules forms the basis of understanding their function and their mechanism of action. It also lays the foundation for rational protein and drug design. The only method to obtain this knowledge is still crystallography. At present, the structures of about 400 proteins are known at or nearly at atomic proteins. However, only two of them are membrane proteins or complexes of the membrane proteins. The reasons for the difference is not the crystals of membrane proteins resists forming special problems when being analysed. The reason is that the membrane proteins resist into forming into well-ordered crystals. The intention of this book is to help to produce

well-ordered crystals proteins and to provide guidelines, it is aimed at both biochemists and protein crystallographer‘s.
The concept of reciprocal space is over 100 years old, and has been of particular use by crystallographers in order to understand the patterns of spots when x-rays are diffracted by crystals. However, it has a much more general use, especially in the physics of the solid state. In order to understand what it is, how to construct it and how to make use of it, it is first necessary to start with the so-called real or direct space and then show how reciprocal space is related to it. Real space describes the objects we see around us, especially with regards to crystals, their physical shapes and symmetries and the arrangements of atoms within: the so-called crystal structure. Reciprocal space on the other hand deals with the crystals as seen through their diffraction images. Indeed, crystallographers are accustomed to working backwards from the diffraction images to the crystal structures, which we call crystal structure solution. In solid state physics, one usually works the other way, starting with reciprocal space to explain various solid-state properties, such as thermal and electrical phenomena. In this book, I start with the crystallographer's point of view of real and reciprocal space and then proceed to develop this in a form suitable for physics applications. Note that while for the crystallographer reciprocal space is a handy means of dealing with diffraction, for the solid-state physicist it is thought of as a way to describe the formation and motion of waves, in which case the physicist thinks of reciprocal space in terms of momentum or wave-vector k-space. This is because, for periodic structures, a characteristic of normal crystals, elementary quantum excitations, e.g. phonons and electrons, can be described both as particles and waves. The treatment given here, will be by necessity brief, but I would hope that this will suffice to lead the reader to build upon the concepts described. I have tried to write this book in a suitable form for both undergraduate and graduate students of what today we call "condensed matter physics."
The book presents the basic information needed to understand and to organize the huge amount of known structures of crystalline solids. Its basis is crystallographic group theory (space group theory), with special emphasis on the relations between the symmetry properties of crystals.
The Brief Teaching Edition of International Tables for Crystallography Volume A is a handy and inexpensive tool for researchers and students wishing to familiarize themselves with the use of the space-group tables in Volume A. This condensed, inexpensive version of Volume A consists of: (i) complete descriptions of the 17 plane groups, useful for the teaching of symmetry; (ii) 24 selected space-group examples, of varying complexity and distributed over all seven crystal systems; (iii) those basic text sections of Volume A that are necessary for the understanding and handling of space groups. This volume is designed for use in classroom teaching, and also serves as a useful laboratory handbook because the 24 examples include most of the frequently occurring space groups, for both organic and inorganic crystals.

The present volume treats the symmetries on one-, two- and three-dimensional space groups and point groups in direct space. New features in this edition include additional data and diagrams in the space-group tables and an extension of the synoptic tables.

International Tables for Crystallography are no longer available for purchase from Springer. For further information please contact Wiley Inc. (follow the link on the right hand side of this page). Volume B presents accounts of the numerous aspects of reciprocal space in crystallographic research. After an introductory chapter, Part 1 presents the reader with an account of structure-factor formalisms, an extensive treatment of the theory, algorithms and crystallographic applications of Fourier methods, and fundamental as well as advanced treatments of symmetry in reciprocal space. In Part 2, these general accounts are followed by detailed expositions of crystallographic statistics, the theory of direct methods, Patterson techniques, isomorphous replacement and anomalous scattering, and treatments of the role of electron microscopy and diffraction in crystal structure determination, including applications of direct methods to electron crystallography. Part 3 deals with applications of reciprocal space to molecular geometry and `best'-plane calculations, and contains a treatment of the principles of molecular graphics and modelling and their applications. A convergence-acceleration method of importance in the computation of approximate lattice sums is presented and the part concludes with a discussion of the Ewald method. Part 4 contains treatments of various diffuse-scattering phenomena arising from crystal dynamics, disorder and low dimensionality (liquid crystals), and an exposition of the underlying theories and/or experimental evidence. Polymer crystallography and reciprocal-space images of aperiodic crystals are also treated. Part 5 of the volume contains introductory treatments of the theory of the interaction of radiation with matter (dynamical theory) as applied to X-ray, electron and neutron diffraction techniques. The simplified trigonometric expressions for the structure factors in the 230 three-dimensional space groups, which appeared in Volume I of International Tables for X-ray Crystallography, are now given in Appendix 1.4.3 to Chapter 1.4 of this volume. Volume B is a vital addition to the library of scientists engaged in crystal structure determination, crystallographic computing, crystal physics and other fields of crystallographic research. Graduate students specializing in crystallography will find much material suitable for self-study and a rich source of references to the relevant literature.

International Tables for Crystallography is the definitive resource and reference work for crystallography and structural science. Volume B presents accounts of the numerous aspects of reciprocal space in crystallographic research. This volume is a vital addition to the library of scientists engaged in crystal structure determination, crystallographic computing, crystal physics and other fields of crystallographic research. Graduate students specializing in crystallography will find much material suitable for self-study and a rich source of references to the relevant literature. New to this edition: A new chapter on modern extensions of the Ewald method for Coulomb interactions in crystals. Three new sections on electron diffraction and electron microscopy in structure determination, describing point-group and space-group determination by convergent-beam electron diffraction, three-dimensional reconstruction, and single-particle reconstruction. Substantial revisions to the chapters on space-group representations in reciprocal space, direct methods, Patterson and molecular replacement techniques, and disorder diffuse scattering More information on the series can be found at: http://it.iucr.org

International Tables for Crystallography is the definitive resource and reference work for crystallography and structural science. Now in nine volumes, each of the volumes in the series contains articles and tables of data relevant to crystallographic research and to applications of crystallographic methods in all sciences concerned with the structure and properties of materials. Emphasis is given to symmetry, diffraction

methods and techniques of crystal-structure determination, and the physical and chemical properties of crystals. The data are accompanied by discussions of theory, practical explanations and examples, all of which are useful for teaching. The contents can be browsed by volume, across the 9 volumes below: Volume A: Space-group symmetry, 5e Volume A1: Symmetry relations between space groups Volume B: Reciprocal space, 3e Volume C: Mathematical, physical and chemical tables, 3e Volume D: Physical properties of crystals Volume E: Subperiodic groups Volume F: Crystallography of biological macromolecules Volume G: Definition and exchange of crystallographic data Volume H: Powder Diffraction Also available online as an updating reference representing the most up-to-date, dynamic, and comprehensive reference work available to crystallographers, and to all those who use crystallography across a wide range of fields.

A fresh approach to teaching crystallographic symmetry. Rather than being swamped by heavy algebraic notation, the reader is taken through a series of simple and beautiful examples from the visual arts, and taught how to analyse them employing the 'pictorial' diagrams used in the International Tables of Crystallography.

This book provides a clear introduction to topics which are essential to students in a wide range of scientific disciplines but which are otherwise only covered in specialised and mathematically detailed texts. It shows how crystal structures may be built up from simple ideas of atomic packing and co-ordination, it develops the concepts of crystal symmetry, point and space groups by way of two dimensional examples of patterns and tilings, it explains the concept of the reciprocal lattice in simple terms and shows its importance in an understanding of light, X-ray and electron diffraction. Practical examples of the applications of these techniques are described and also the importance of diffraction in the performance of optical instruments. The book is also of value to the general reader since it shows, by biographical and historical references, how the subject has developed and thereby indicates some of the excitement of scientific discovery.

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This volume contains tables on the 17 plane groups and 230 space groups and is complemented by a comprehensive introduction in which symmetry is discussed and the theory and use of the tables is described in detail. This fourth edition incorporates new diagrams for all plane groups and space groups.